REPORT DOCUMENTATION PAGE

Form Approved
OMB NO. 0704-0188

1. AGENCY USE ONLY (Leave Blank)	2. REPORT DATE	3. REPORT TYPE AND DATES COVERED
	November 30, 2004	6/1/01-8/31/04; Final Progress Rep

4. TITLE AND SUBTITLE
High-Order Accuracy Methods for the Modeling & Design of Microoptics & Phototonic Devices

5. FUNDING NUMBERS
DAAD19-01-1-0631

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3

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)
U. S. Army Research Office
P.O. Box 12211
Research Triangle Park, NC 27709-2211

10. SPONSORING / MONITORING AGENCY REPORT NUMBER
40464.6-MA

11. SUPPLEMENTARY NOTES
The views, opinions and/or findings contained in this report are those of the author(s) and should not be construed as an official Department of the Army position, policy or decision, unless so designated by other documentation.

12 a. DISTRIBUTION / AVAILABILITY STATEMENT	12 b. DISTRIBUTION CODE
Approved for public release; distribution unlimited.	

13. ABSTRACT (Maximum 200 words)
The goals of this effort has been the development of high-order accurate computationl methods for wave problems in general and Maxwell's equations of electromagnetics in particular. The applications are general but particular emphasis has been on optical applications.
We have obtained substantial progress in the development and application of three different methods: embedded high-order finite difference methods, boundary variation methods, and discontinuous Galerkin methods for the harmonic Maxwell equation.

14. SUBJECT TERMS	15. NUMBER OF PAGES 6
	16. PRICE CODE

17. SECURITY CLASSIFICATION OR REPORT	18. SECURITY CLASSIFICATION ON THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
UNCLASSIFIED	**UNCLASSIFIED**	**UNCLASSIFIED**	**UL**

NSN 7540-01-280-5500

Standard Form 298 (Rev.2-89)
Prescribed by ANSI Std. 239-18
298-102

Enclosure 1

Final Progress Report – DAAD19-01-1-0631

Purpose and Goals of Effort

The overarching goals of this effort has been the continued development of high-order accurate computational methods for wave problems in general and Maxwell's equations of electromagnetics in particular. The applications are general but particular emphasis has been on optical applications.

Rather than focusing on one particular approach, we have pursued such developments along three different directions

- *Time-Domain High-order Embedding Methods* Focuses on the development, analysis, and implementation of a 4th order finite difference embedded interface scheme for the time-domain solution of Maxwell's equations. This enables the solution of geometrically complex problems, including real materials, using a Cartesian grid without sacrificing accuracy, stability and robustness. Part of this also requires attention to related issues such a efficient and robust absorbing boundary conditions.
- *Boundary Variation Methods for Multilayered Optics* Focuses on boundary variation techniques for the solution of Maxwell's equations in the frequency domain. Applications are taken from photonics and integrated optics, including waveguide couplers, multilayer devises, and transmission and reflection diffractive optics.
- *DG-FEM Methods for the Harmonic Maxwell Problem* Focuses on the development and analysis for Discontinuous Galerkin Methods for the harmonic frequency domain Maxwell problem as well as the wave Helmholtz problem. These are generic methods, the details of which are still poorly understood and we have developed the analysis and computational tools in parallel. Subtle issues such as spuriuos modes and efficient preconditioning techniques for the resulting indefinite linear systems.

Overview of Main Results

In the following we shall discuss these efforts in some more detail, highligthing the progress made during this effort as reported in the publications.

Embedded Interface Methods

Within the scope of this research, we have achieved the following most notable tasks

- Following previous pioneering work by us, we have developed 4th order accurate finite difference schemes which are able to solve wave problems stated in complex geometries. This development overcomes classic problems of staircasing and the effect internal boundaries in a unified way. As the scheme is modified locally only, it maintains the simplicity and computational efficiency of the original formulation as most of the additional work, i.e., computing the local schemes, is done in a preprocessing stage.

The extension of these ideas to 4th order embedding methods is far from trivial. However, we have succeeded in formulating and implementing such a scheme, using a standard staggered grid everywhere in space and locally modifying the scheme by use of one sided stencils and extrapolations.

Computational experimentation and preliminary analysis confirms the stability of the embedding scheme for situations where the material interfaces are straight. The scheme is currently being implemented and tested in a two-dimensional version, with preliminary results being very encouraging.

The scheme is currently being implemented in a production code for use on DoD-related applications.

- We have investigated some long time stability problems observed in PML methods used for absorbing waves in the time-domain schemes. Extensive computations showed the potential for weak instability and the source of this was found to be in the degenerate low-order terms. This understanding enabled stabilization by breaking the degeneracy.

- We have proposed an entirely new family of absorbing layer methods of a nonlinear nature – known as nonlinear PML methods. These are perfectly matched layers, yet require no additional variables, thus reducing the memory usage signifcantly. The analysis of this scheme remains incomplete due to its nonlinear nature but computational results very encouarging.

Boundary Variation Methods

Within the scope of this research, we have achieved the following most notable tasks

- A first goal was to finalize work on the development of three-dimensional boundary variation methods for single interface scattering, in particular with applications to waveguide couplers.

  This has been accomplished as planned and several large scale applications has been completed.

- As a second goal, we have developed an entirely new class of boundary variation methods for multilayered transmission optics.

  A flexible and fast approach for the two-dimensional harmonic problem has been developed. The algorithm relies on recursive use of a highly optimized one-layer scheme and allows the modeling of an arbitrary number of dielectric layers, each with an interface of arbitrary shape. Important special cases include the ability to model transmission optics of finite extend and problems illuminated by beams.

  A key development is the use of physical insight to enable a fast and cost effective of the recursive approach. With out relying on the physical properties of the scattering and diffraction processes, the recursive process would grow exponentially in

complexity. With this new formulation, the growth is bounded from above and all central components are precomputed.

The developed software has been validated carefully by comparison with selected exact solutions as well as by careful cross validation of results obtained using the high-order time-domain codes. Extensions to the three-dimensional vectorial case is expected to be relatively straightforward, based on the general algorithmic developments.

- The methods for fast and accurate modeling of multilayered diffractive optics have been validated and used extensive by several research groups, e.g., at Bell Labs for studies of the impact of roughness in Bragg mirrors in lasers and at the National Lab of Denmark to model and design highly sensitive sensors for measuring bacterial content in liquids. These collaborations have both led to further developments of the algorithm as well as facilitated an increased understanding and analysis of the particular applications at hand. The results of both efforts are being prepared for publication.

- In a closely related effort we have demonstrated the use of the boundary variation method as a tool to analyze errors coming with poor geometry-descriptions in standard finite-difference schemes used for solving Maxwell's equations. The boundary variation method allows for solving the diffraction problem, appearing by representing a straight interface by a stair-cased approximation, exactly, hence providing a mechanism to separate discretization errors from errors from geometry descriptions. The results show that the physics of the problems changes dramatically and one can only expect first order convergence in amplitude and phase computed fields. This is indeed a strong argument for why embedded interface methods are needed.

DG-FEM Methods for the Harmonic Maxwell Problem

Within the scope of this research, we have achieved the following most notable tasks

- we We have initiated the investigation of the ability to accurately and efficiently approximate eigenvalue problems originating in Maxwell's equations, i.e., when computing eigenmodes of resonators. This is a notoriously hard problem due to the nature of the curl-curl form of Maxwell's equations and the associated boundary conditions.

  The emphasis has been on the possibility of accurately and reliably solve the eigenvalue problem for nonsmooth geometries where the eigensolutions can exhibit strong singularities.

  The computional approach is that of high-order discontinuous Galerkin methods on fully unstructured grid. Such methods has not been explored in detail for Maxwell eigenvalue problems previously and our study analysis has revealed some unexpected properties of the discretization, the discrete null space of the operators and ways to stabilize it.

The study has been focused on the possibility of exciting spurious modes, as well-known problem in classical nodal finite element methods, and general behavior. No significant problems of spurious modes have been found, confirming that this formulation is well suited for dealing with geometrically complex nonsmooth problems.

- In the frequency domain we have continued the development of high-order accurate discontinuous Galerkin methods for Maxwell's equations. The schemes are completely general and highly flexible, using arbitrary order and fully unstructured grids.

  Solving the resulting discrete problems is challending for several reasons. The size can very considerable and we must seek techniques that map to parallel computing platforms. Furthermore, the condition number of the matrix scales quite poorly with both the inverse element size and the order of approximation. Finally, the problem is highly indefinite which rules out most standard preconditioning techniques.

  As a prototype problem we are considering the wave Helmholtz problem for which we have developed a two-level additive overlapping Schwarz preconditioner and tested it extensively. In the low frequency case, where the matrix remains definite, this preconditioner complete removes both grid and order dependence, resulting in constant iteration count.

  For the indefinite case, the coarse grid solver becomes essential in reducing the dependence of the iteration count on the wavenumber. However, it does not eliminate it completely as eigenvalues cross the axis when being shifted from coarse to fine grid and back. The number of these grows like the squareroot of the wavenumber and the iteration count scales like this.

  However, this weak dependence is better that most other schemes and the overlapping Schwarz scheme is superior when also taking into account its successful treatment of by grid and order dependence as well as it inherent parallel nature.

  Currently we are extenting these ideas to the full curl-curl form of Maxwell's equations as well as considering the optimization of fluxes and use of multiplication Schwarz methods.

Dissemination Acknowledging Support

Journal Papers (Peer-Reviewed)

- J.S. Hesthaven and T. Warburton, 2004, *High Order Nodal Discontinuous Galerkin Methods for the Maxwell Eigenvalue Problem*, Royal Soc. London Ser A **362**, 493–524.

- L. Wilcox, P. G. Dinesen, and J. S. Hesthaven, 2004, *Fast and Accurate Boundary Variation Method for Multilayered Diffraction Optics*, J. Opt. Soc. Ame. A **21**(5), 757–769.

- J. S. Hesthaven and T. Warburton, 2004, *Discontinuous Galerkin Methods for the Time-Domain Maxwell's Equations: An Introduction*, ACES Newsletter **19**(1), 10–29.
- J. S. Hesthaven and T. Warburton, 2004, *High-Order Accurate Methods for Time-domain Electromagnetics*, Comp. Mod. Engin. Sci. **5**(5), 395–408.
- J. S. Hesthaven, 2003, *High-Order Accurate Methods in Time-Domain Computational Electromagnetics. A Review.* Advances in Imaging and Electron Physics **127**, 59-123.
- T. Warburton and J. S. Hesthaven, 2003, *On the Constants in hp-Finite Element Trace Inequalities*, Comput. Methods Appl. Mech. Engin. **192**, 2765–2773.
- S. Abarbanel, D. Gottlieb, and J. S. Hesthaven, 2002, *Long Time Behavior of the Perfectly Matched Layer Equations in Computational Electromagnetics*, J. Sci. Comput. **17**(1-4), 405-422.

Conference Contributions (Peer-Reviewed)

- A. Ditkowski, K. Dridi, J. S. Hesthaven, and C. H. Teng, 2001, *Embedded FDTD Methods for Maxwell's Equations.* In Fourth International Workshop on Computational Electromagnetics in the Time-Domain: TLM/FDTD and Related Techniques, Nottingham, UK. C. Christopoulos (Eds). pp. 1-6.

Papers Submitted for Peer-Review

- R. Horvath, L.C. Wilcox, H.C. Pedersen, N. Skiversen, J.S. Hesthaven and P.M. Johansen, 2004, *Analytical Theory of Grating Couplers for Waveguide Sensing: A Perturbational Approach and its Limitations*, J. Opt. Soc. Ame. A
- Q. Y. Chen, D. Gottlieb, and J. S. Hesthaven, 2003, *Pseudospectral Methods using Prolate Spheroidal Wavefunctions*, SIAM J. Sci. Comput.
- S. Abarbanel, D. Gottlieb, and J. S. Hesthaven, 2004, *Nonlinear Perfectly Matched Layers*, J. Sci. Comput.
- J.S. Hesthaven, L. Olson, and L. Wilcox, *Overlapping Schwarz Preconditioning for hp-Discontinuous Galerkin Approximations of the Wave Helmholtz Equation*, J. Comput. Phys.

Invited Lectures

Plenary

Recent Advances and Emerging Challenges in Computational Electromagnetics. Spring Meeting of the Swiss Mathematical Society, Basel, Switzerland. 2003.

High-Order Methods in Time-Domain Electromagnetics. Recent Advances and State-of-the-Art in Computational Electromagnetics, Army High Performance Computing Research Center (AHPCRC), Minnesota, MN. 2002.

Workshops

J. S. Hesthaven and T. Warburton, 2004, *High-Order Accurate Time-Domain Solution of Maxwell's Equations in Complex Geometries.* Progress in Electromagnetic Research Symposium, PIERS 2004, Pisa, 2004.

J. S. Hesthaven and T. Warburton 2003, *High Order Nodal DG-FEM for the Maxwell Eigenvalue Problem*, Mafelap 2003, Brunel University, UK, 2003

J. S. Hesthaven, 2001, *Embedded Finite Difference Methods for Wave Problems in Complex Geometries and Heterogeneous Media.* Proc. of 96'th AMS Regional Meeting. Las Vegas, NV. p. 45.

Seminars

Sandia National Laboratory (05/2004); University of North Carolina at Charlotte, Department of Mathematic (04/2004); North Carolina State University, Department of Mathematic (04/2004); University of Wyoming, Department of Mathematic (04/2004);

University of Notre Dame, Department of Mathematic (01/2003); Chalmers University of Technology, Sweden (08/2003); Purdue University, Department of Mathematics (11/2003).

Stanford University, Department of Mathematics (02/2002); Swedish Defense Research Agency, Aeronautics Division, FFA, Sweden (05/2002); University of Basel, Department of Mathematics, Switzerland (06/2002), Chalmers University of Technology, Sweden (09/2002); Massachusetts Institute of Technology, Mechanical Engineering (10/2002); Arizona State University, Department of Mathematics (11/2002); University of Texas, Austin, TICAM (11/2002).

United Technologies Research Center, Hartford (05/2001); Uppsala University, Department of Scientific Computing, Sweden (08/2001); University of Delaware, Department of Mathematical Sciences (10/2001); Carnegie Mellon, Department of Mathematical Sciences (10/2001).

Personnel involved in project

- Jan S. Hesthaven, PI
- Qianyong Chen. Completed PhD 2004.
- Lucas Wilcox. Graduate student, PhD completion expected 2006.